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Title: Leading-Order Analysis by Artificial Intelligence

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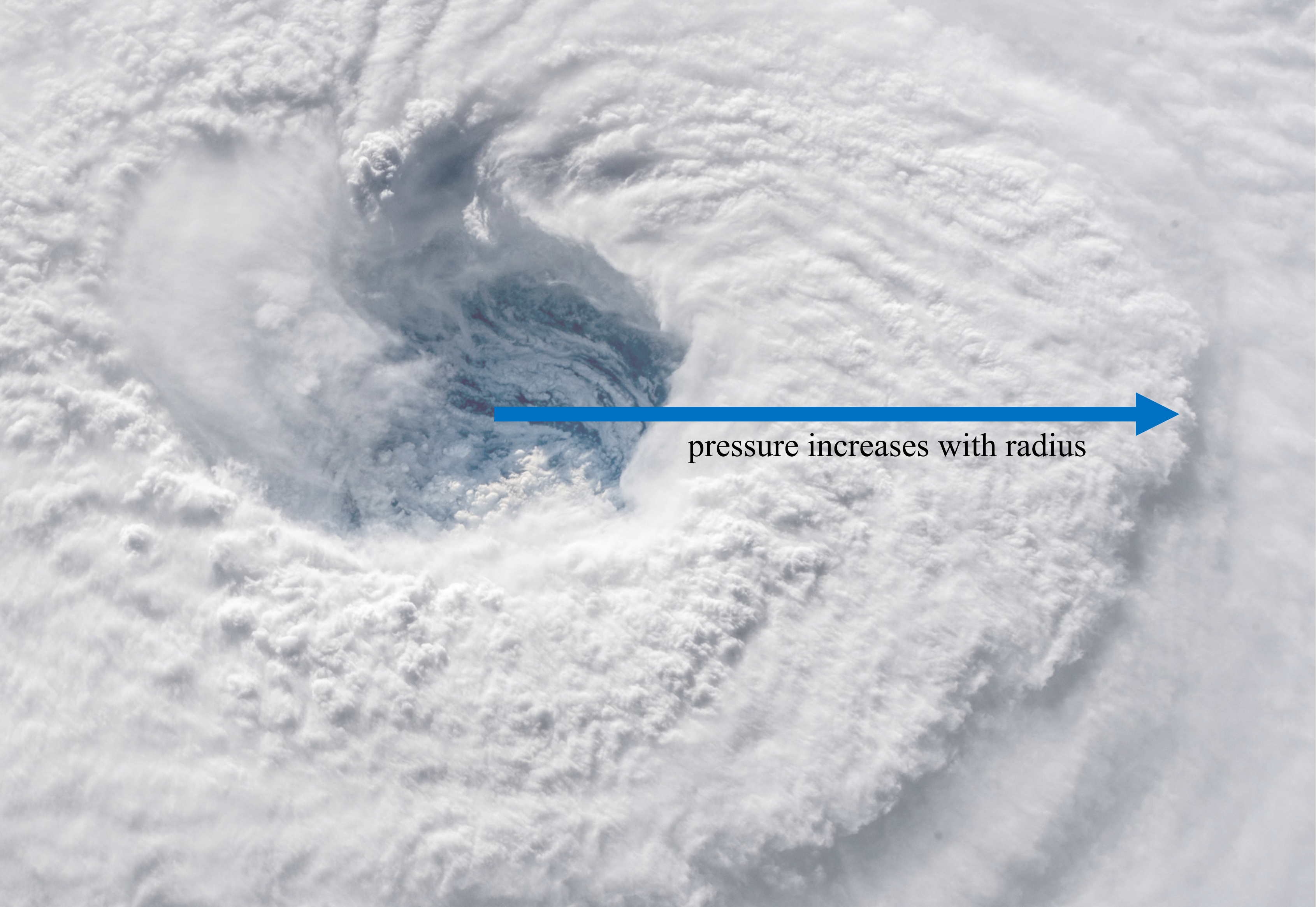
Leading-Order Analysis by Artificial Intelligence

Bryan Kaiser, Juan Saenz, & Daniel Livescu

The eye of hurricane Florence (2018).

Hurricanes "swirl" because the Coriolis force and pressure gradient force balance at leading-order, which causes hurricane winds follow lines of constant pressure (isobars):



Los Alamos
NATIONAL LABORATORY
EST. 1943

Image credit: NASA

Structure of this seminar

1. **My journey** through engineering & science.

2. **What is leading-order analysis?** How important is it in the history of fluid dynamics, among other natural sciences?

3. **What are supervised and unsupervised machine learning and what is artificial intelligence?**

4. **AI algorithm:** an algorithm and scoring metric for leading-order analysis by AI

5. **Results**

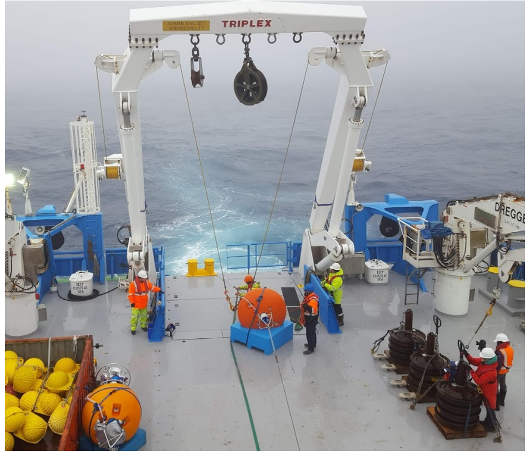
6. **Conclusions & outlook**

Image credit: NASA

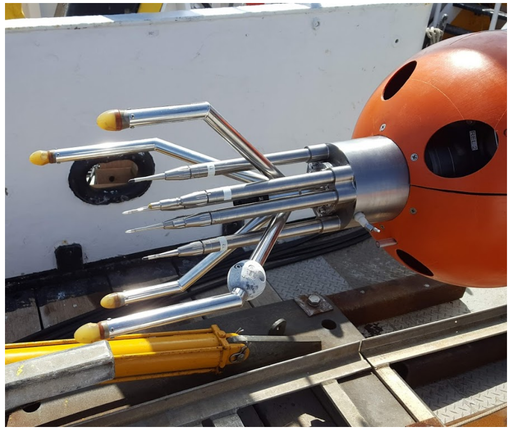
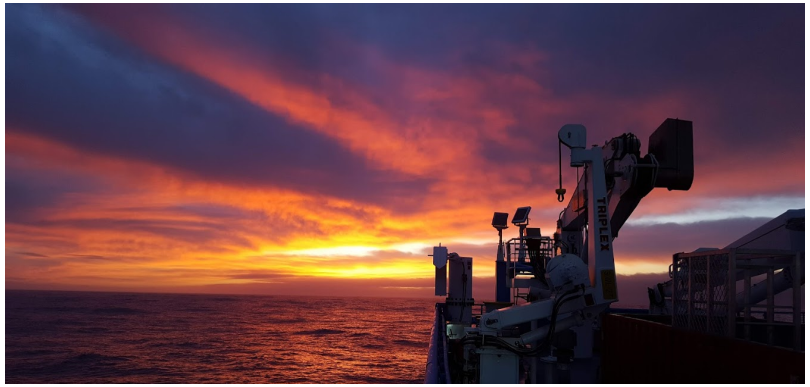
My journey

BSME, MSME
UNM
Advisor: Prof. Svetlana Poroseva

PhD in Physical Oceanography
MIT - Woods Hole Oceanographic Institution Joint Program
Advisor: Larry Pratt





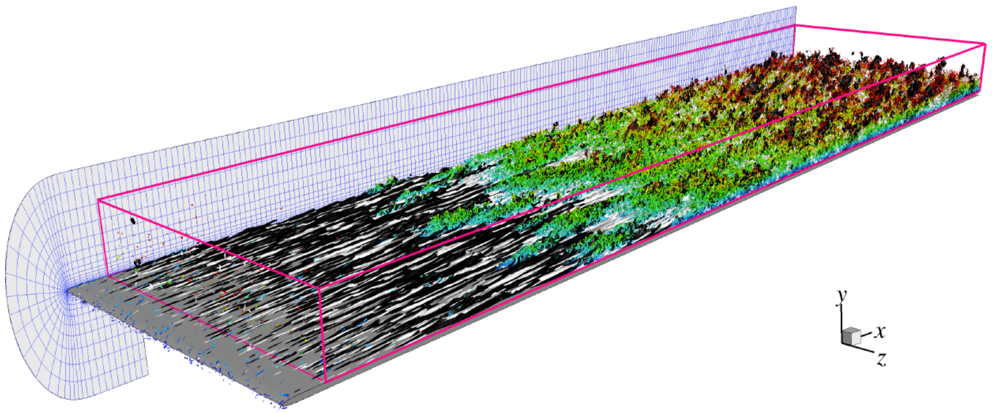
2. What is leading-order analysis?

D'Alembert's paradox (1752)

Since the frictional forces within typical aero/hydrodynamical flows are typically negligibly small, those forces can be neglected everywhere. Therefore *the flow over an immersed body* (e.g. airfoil) *should produce no drag forces*.

Prandtl (1904)

Drag occurs at the surface of immersed bodies because friction is *important* (meaning: *leading-order*) within a thin boundary layer close to the surface of the body.



Transitional boundary layer. The colored isosurfaces delineate the a constant rate of change of vorticity.
Image credit: JHU turbulence database,

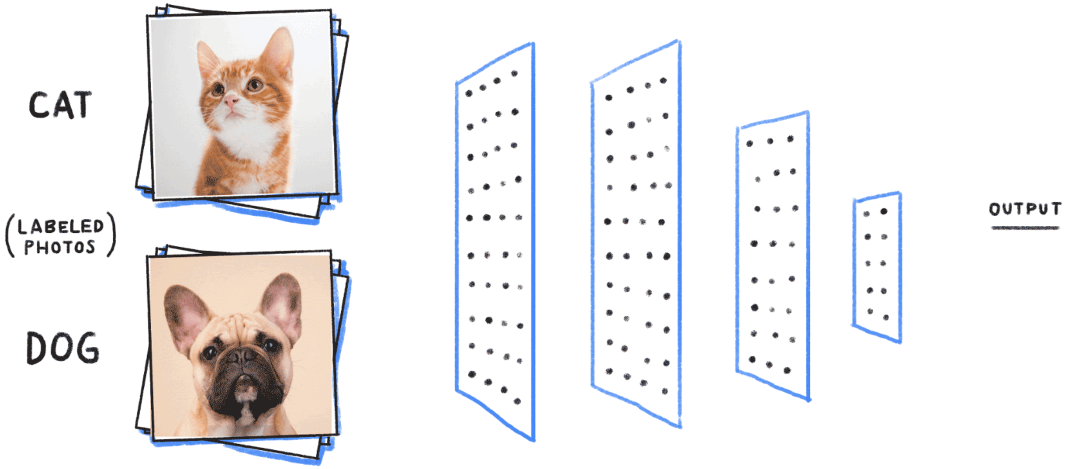
Leading-order analysis includes several (closely related / overlapping) ideas for simplifying equations:

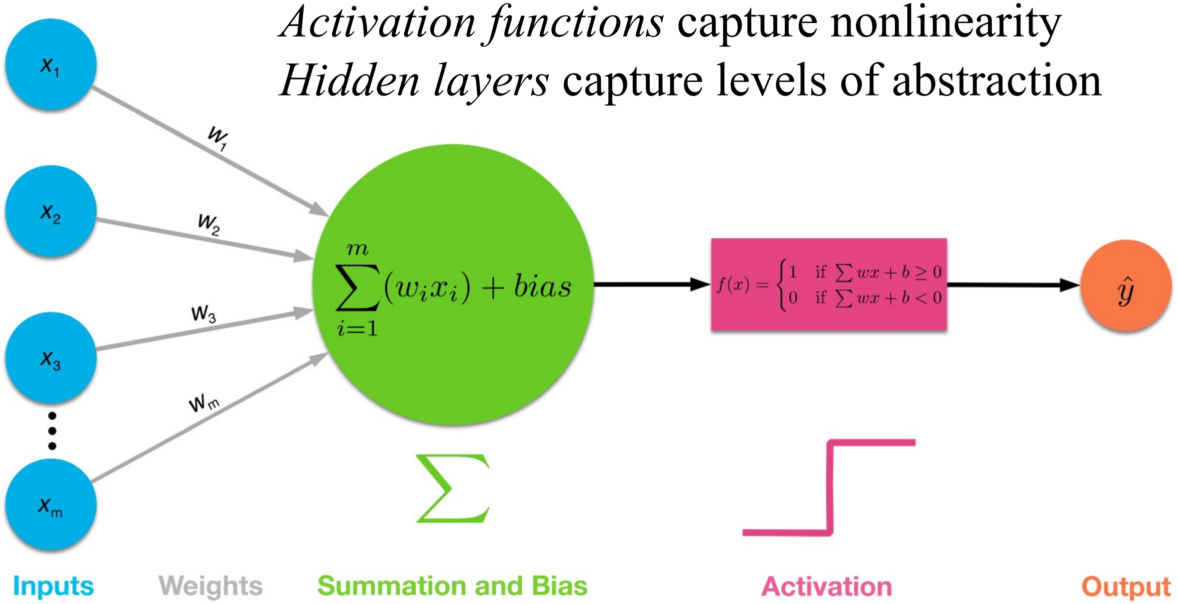
- *Perturbation theory:* truncated series expansions of non-dimensionalized variables / equations / perturbations can be used to eliminate equation terms or discover perturbation dynamics by examining the limits of non-dimensional variables.
- *Method of matched asymptotic expansions:* analytically match solutions at domain interfaces to satisfy disparate boundary conditions (if this is possible, the behavior of the variable is said to be in the "asymptotic regime").
- *Order-of-magnitude analysis:* use characteristic scales from observations to eliminate equation terms through the magnitude of non-dimensional coefficients.

3. Supervised machine learning

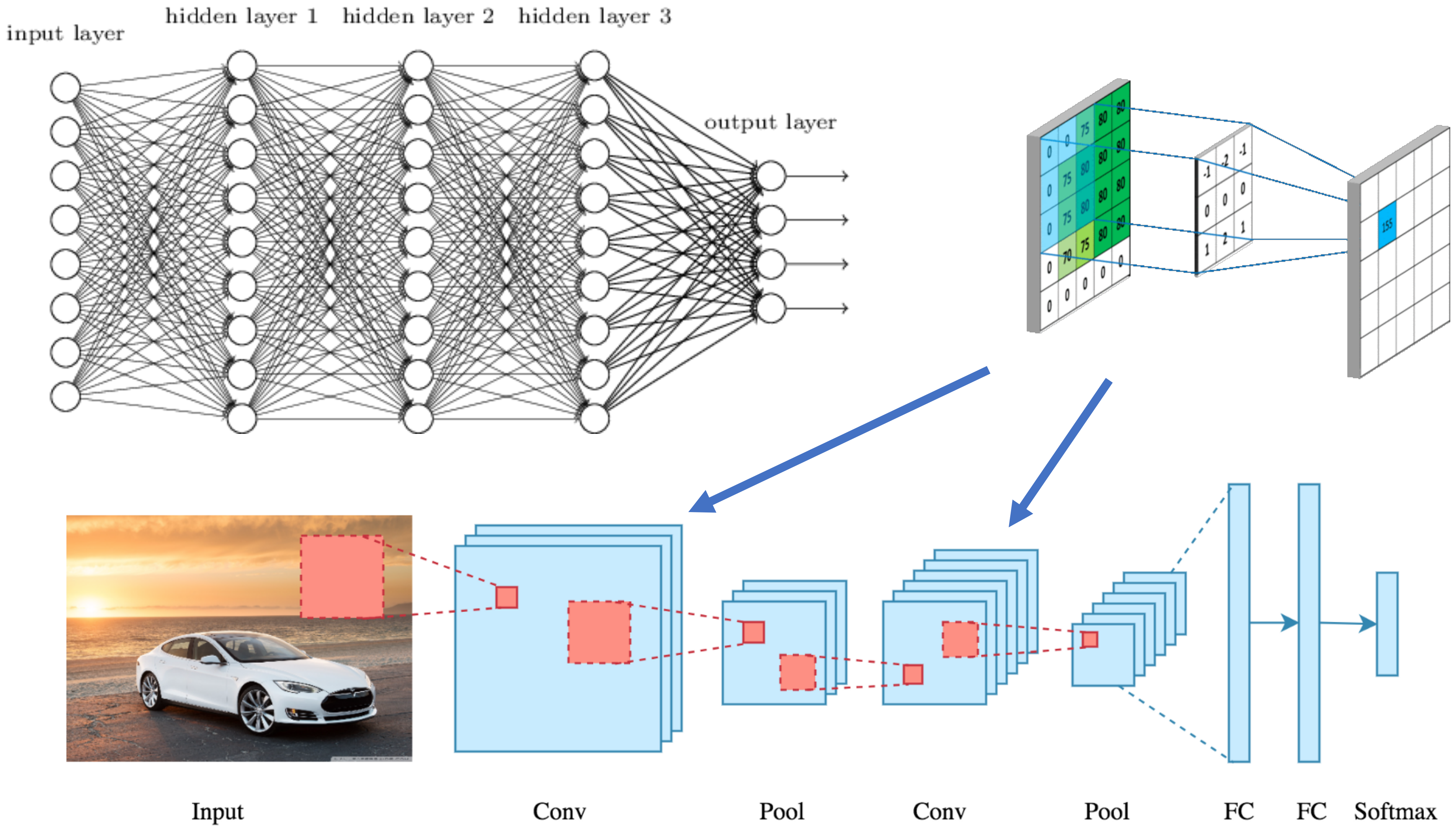
A feature vector, **X**, is fed into a neural network, to obtain the outcome **y**. The ``true'' **y** is known (labels), so the weights of the neural network can be nudged towards lower error with respect to the true **y** (backpropagation). After many nudges the error converges and there is *hopefully* a good fit.

Activation functions capture nonlinearity
Hidden layers capture levels of abstraction



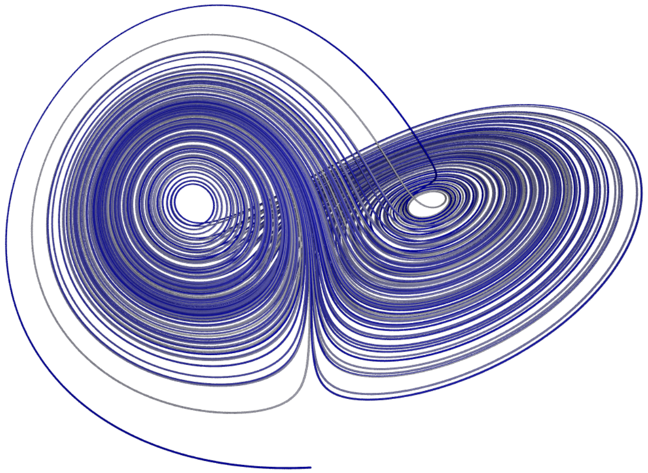


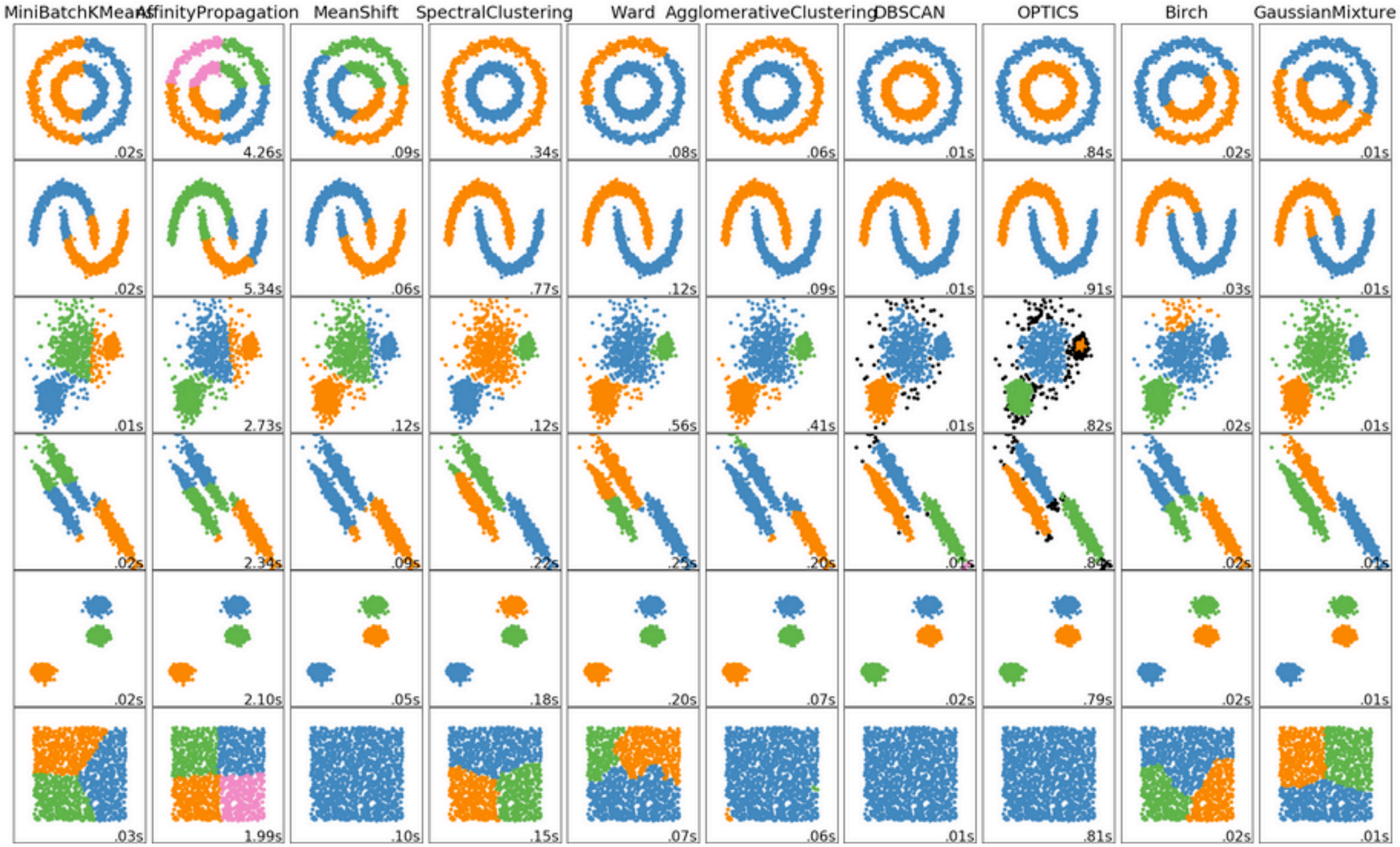
3. Supervised machine learning



3. Unsupervised machine learning

A feature vector, **X**, is fed into a clustering algorithm which then finds clusters in N dimensional space (where N is the number of features) by a stochastic process for optimization or minimization, the details of which depend on the choice of clustering algorithm.





A comparison of the clustering algorithms in scikit-learn

3. Artificial Intelligence

Machine Learning:
Algorithms that generate a prediction or outcome which improves through experience.

Artificial Intelligence:
Algorithms that mimic functions of the human mind, such as *the scientific method*.

The Scientific Method:
1. Formulate a question
2. Formulate a hypothesis
3. Test the hypothesis
4. Analyze the test results

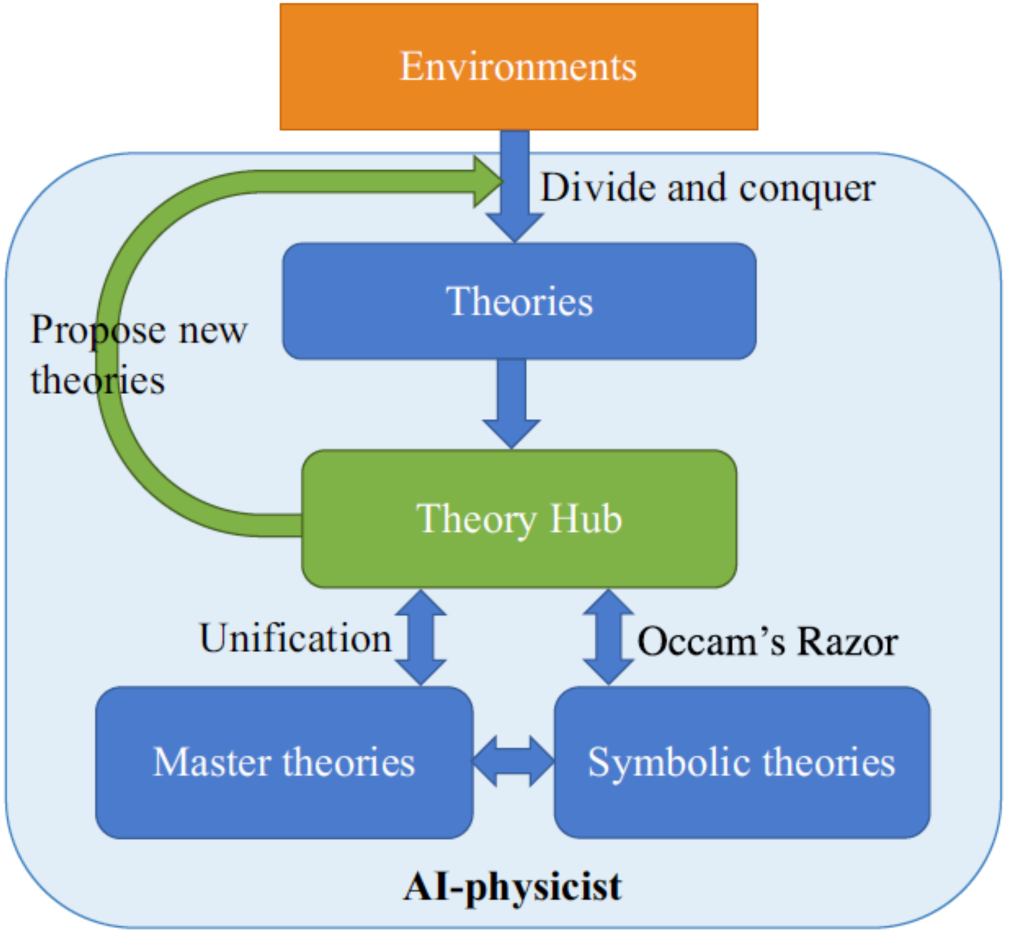
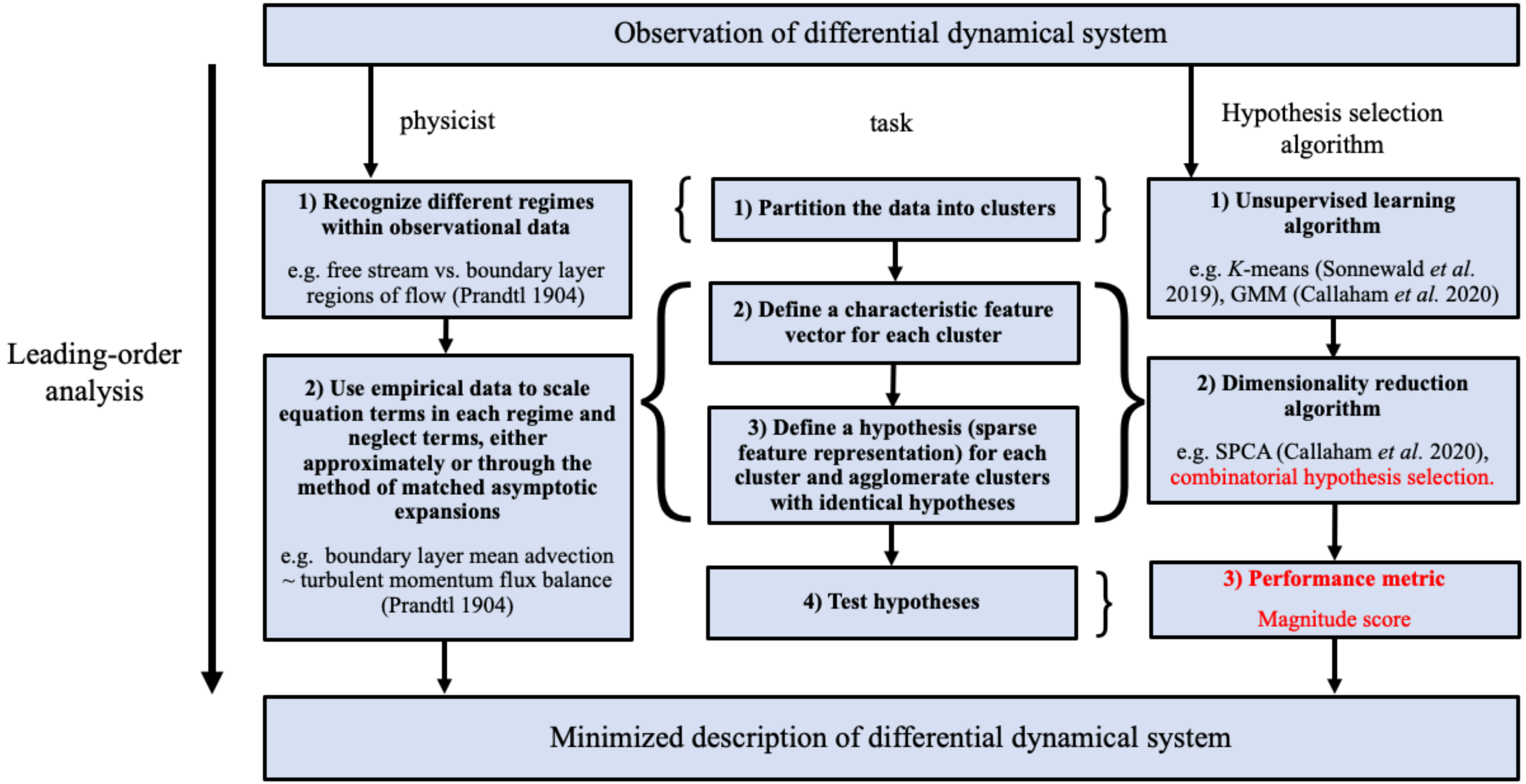


FIG. 1. AI physicist architecture.

Diagram credit: Wu & Tegmark (2019)

4. AI algorithm: replicating the scientific method



4. AI algorithm: magnitude score

3) Performance metric
Magnitude score

Basic idea: using a score that ranks how well a chosen set of equation terms leads the remaining equation terms, select the best set of equation terms (or not, if there are no leading order terms). Each chosen set of equation terms is a hypothesis, which will be tested calculating the score for that chosen set using the data.

Example feature vector:

$$\mathbf{X} = \left[\frac{\partial u}{\partial t}, u\frac{\partial u}{\partial x}, v\frac{\partial u}{\partial y}, w\frac{\partial u}{\partial z}, fv, \frac{1}{\rho}\frac{\partial p}{\partial x}, \nu\frac{\partial^2 u}{\partial x^2}, \nu\frac{\partial^2 u}{\partial y^2}, \nu\frac{\partial^2 u}{\partial z^2}\right],$$

Log of the absolute relative differences w.r.t. the absolute maximum in the set of features:

$$\Delta^d = \log_{10}\left(\frac{|X^p| - |X^d|}{|X^p| + |X^d|}\right) \in (-\infty, 0),$$

Ratio of summed relative differences:

$$s_q = \sum_{i \in d_q} \Delta^i. \qquad s_m = \sum_{i \in d_m} \Delta^i. \qquad \mathcal{R} = \frac{s_q}{s_m} \in (0, 1],$$

Introduce a bias coefficient, which provides a bias towards chosen sets with fewer terms:

$$\mathcal{B} = \frac{N_q}{2(N_q - 1)}, \qquad \lim_{N_q \to \infty} \mathcal{B} = \frac{1}{2}, \qquad \lim_{N_q = 2} \mathcal{B} = 1.$$

The magnitude score:

$$\mathcal{M} = \mathcal{R}\mathcal{B} \in (0, 1].$$

Full set score: $\mathcal{M} = \dfrac{N_m}{2(N_m - 1)},$

4. AI algorithm: combinatorial hypothesis selection

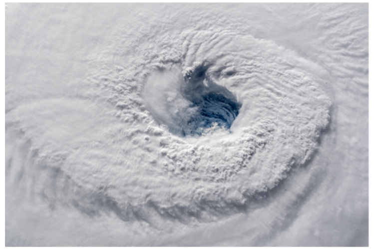
2) Dimensionality reduction algorithm

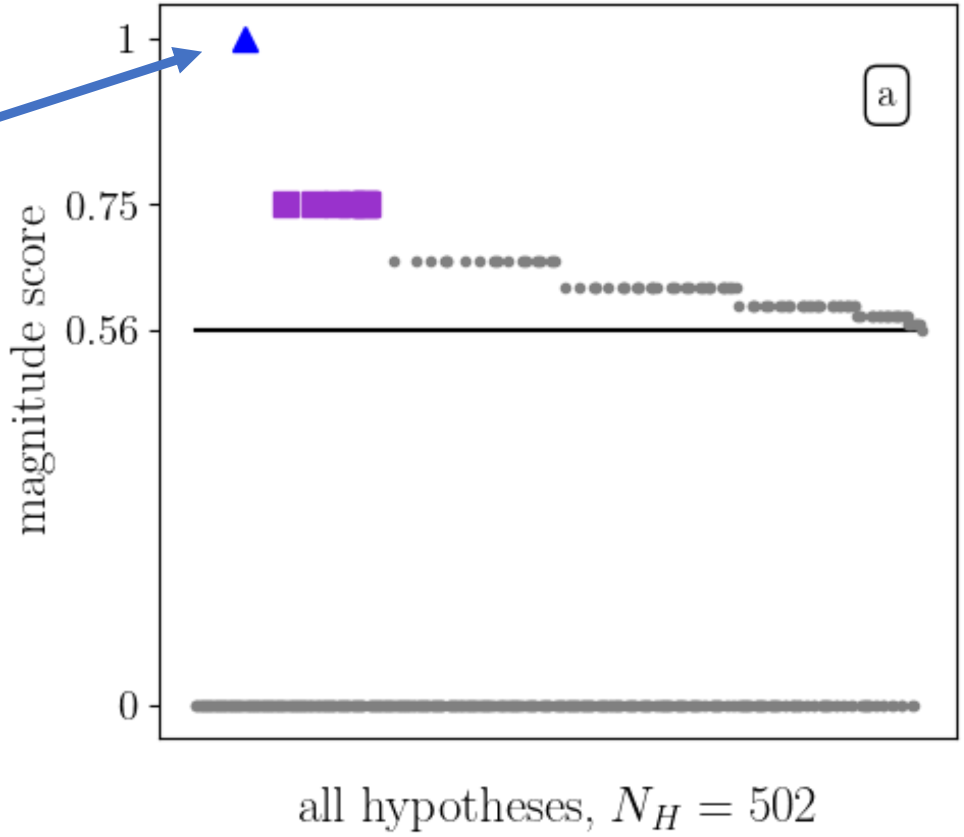
e.g. SPCA (Callaham *et al.* 2020), combinatorial hypothesis selection.

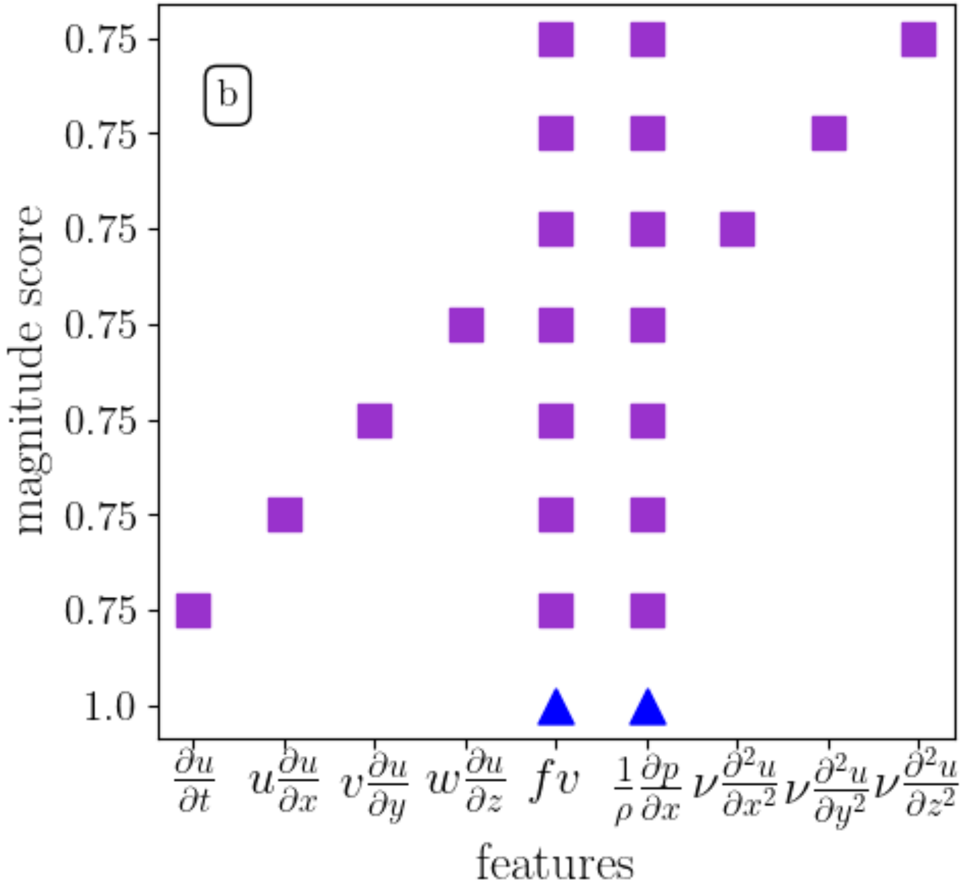
Feature vector, oceanic values at 10^3 km scale:

$$\mathbf{X} \sim \left[\frac{U}{T}, \frac{U^2}{L}, \frac{UV}{L}, \frac{UW}{D}, fV, \frac{P}{\rho L}, \frac{\nu U}{\rho L^2}, \frac{\nu U}{\rho L^2}, \frac{\nu U}{\rho D^2}\right]$$
$$\sim [10^{-10}, 10^{-10}, 10^{-10}, 4 \cdot 10^{-13}, 10^{-6}, 10^{-6}, 10^{-23}, 10^{-23}, 6.25 \cdot 10^{-19}].$$

Geostrophy is selected!







Number of hypotheses: $N_H = 2^{N_m} - 1 - N_m,$

4. AI algorithm: combinatorial hypothesis selection

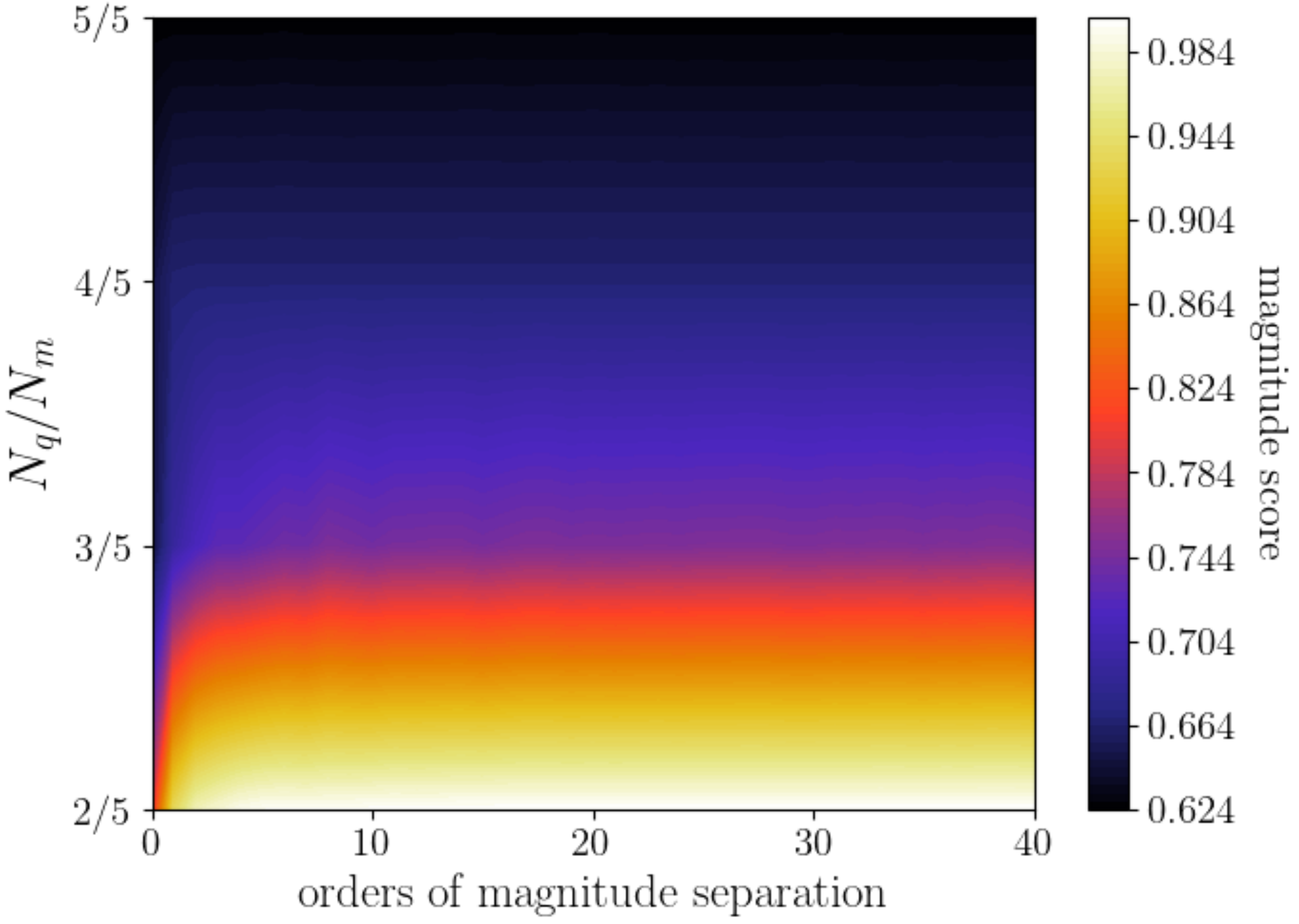
Synthetic data:

Randomly generated equations that *close* with N_m= 5 features (equation terms) and 2 to 5 leading-order term balances, leading by 1 to 40 orders of magnitude. The best score (correct subset selected every time) is plotted:

Full set score for N_m= 5 is 5/8 = 0.6

$$\mathcal{M} = \frac{N_m}{2(N_m - 1)},$$

The best score converges for leading-order terms that **lead by about least three order of magnitude**:



5. Results: transitional boundary layer

Reynolds-averaged boundary layer equations:

$$\mathbf{X} = \left[\overline{u}\frac{\partial \overline{u}}{\partial x}, \overline{v}\frac{\partial \overline{u}}{\partial y}, \frac{1}{\rho}\frac{\partial \overline{p}}{\partial x}, \nu\nabla^2\overline{u}, \frac{\partial \overline{u'v'}}{\partial y}, \frac{\partial \overline{u'^2}}{\partial x}\right],$$

$$\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2,$$

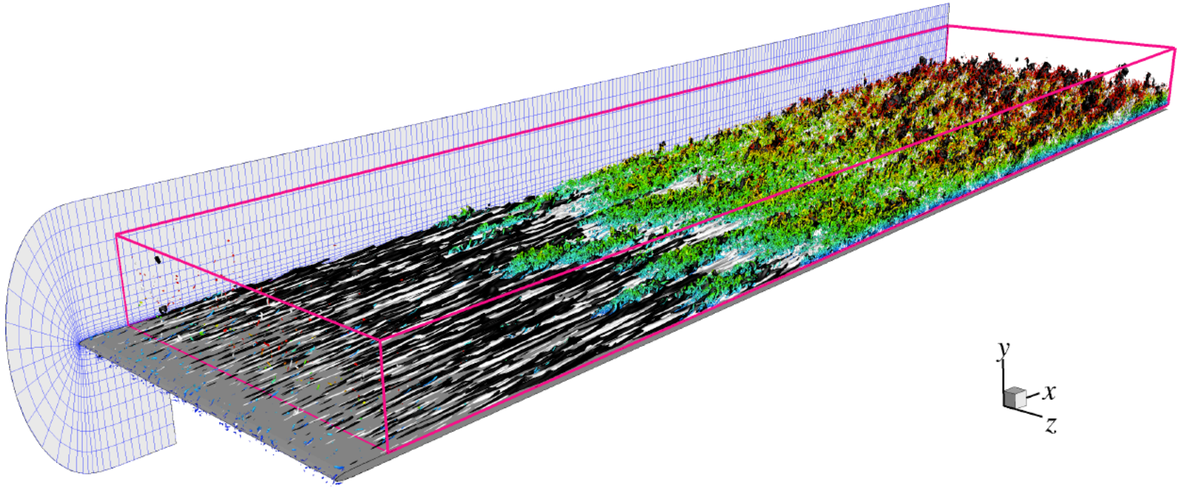


Image credit: JHU turbulence database, transitional boundary layer.

Set free parameters, cluster:

1) Unsupervised learning algorithm

e.g. *K*-means (Sonnewald *et al.* 2019), GMM (Callaham *et al.* 2020)

Identify balances within clusters, combine identical clusters:

2) Dimensionality reduction algorithm

e.g. SPCA (Callaham *et al.* 2020), combinatorial hypothesis selection.

Evaluate area-weighted score for all clusters:

3) Performance metric

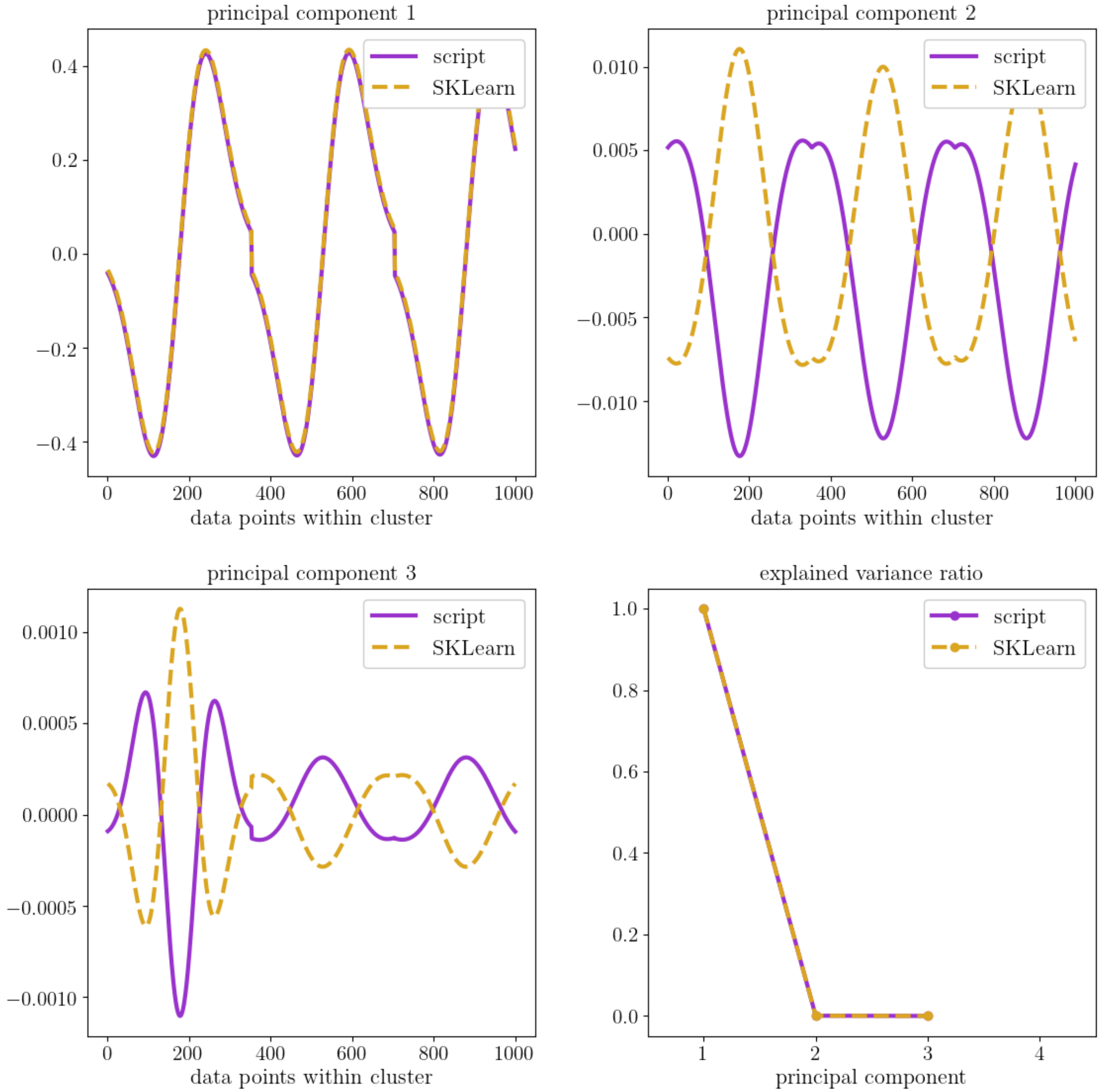
Magnitude score

Loop back to top: repeat for new free parameters

5. Results: why not just use SPCA?

SPCA introduces another free parameter, the LASSO regression coefficient

Principal Component Analysis (PCA) + LASSO regression = Sparse PCA



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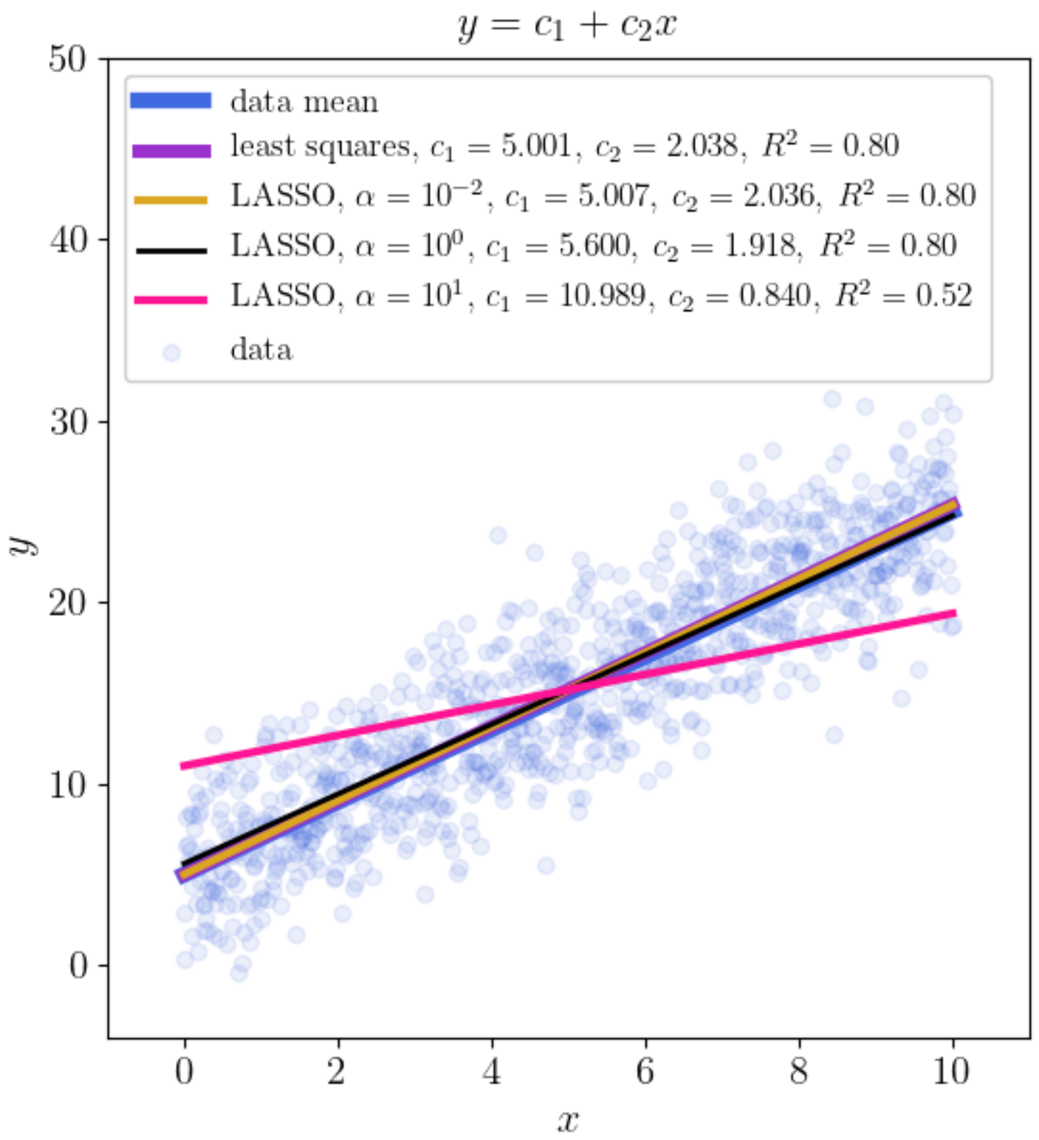
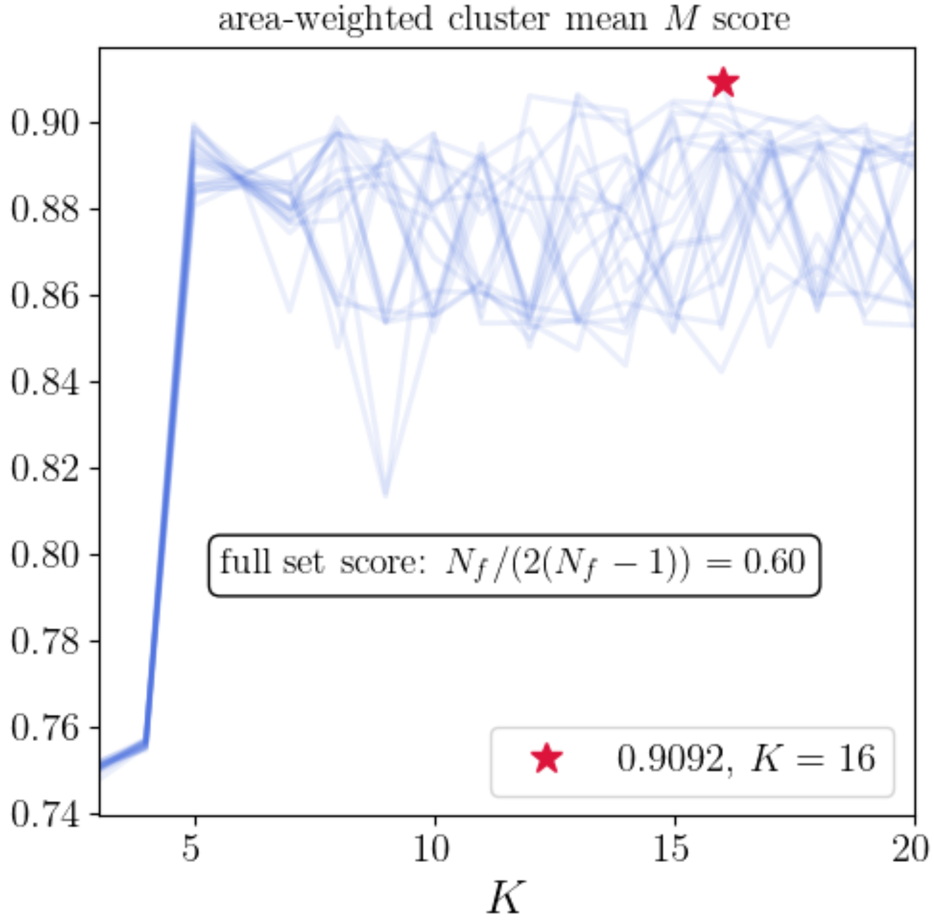
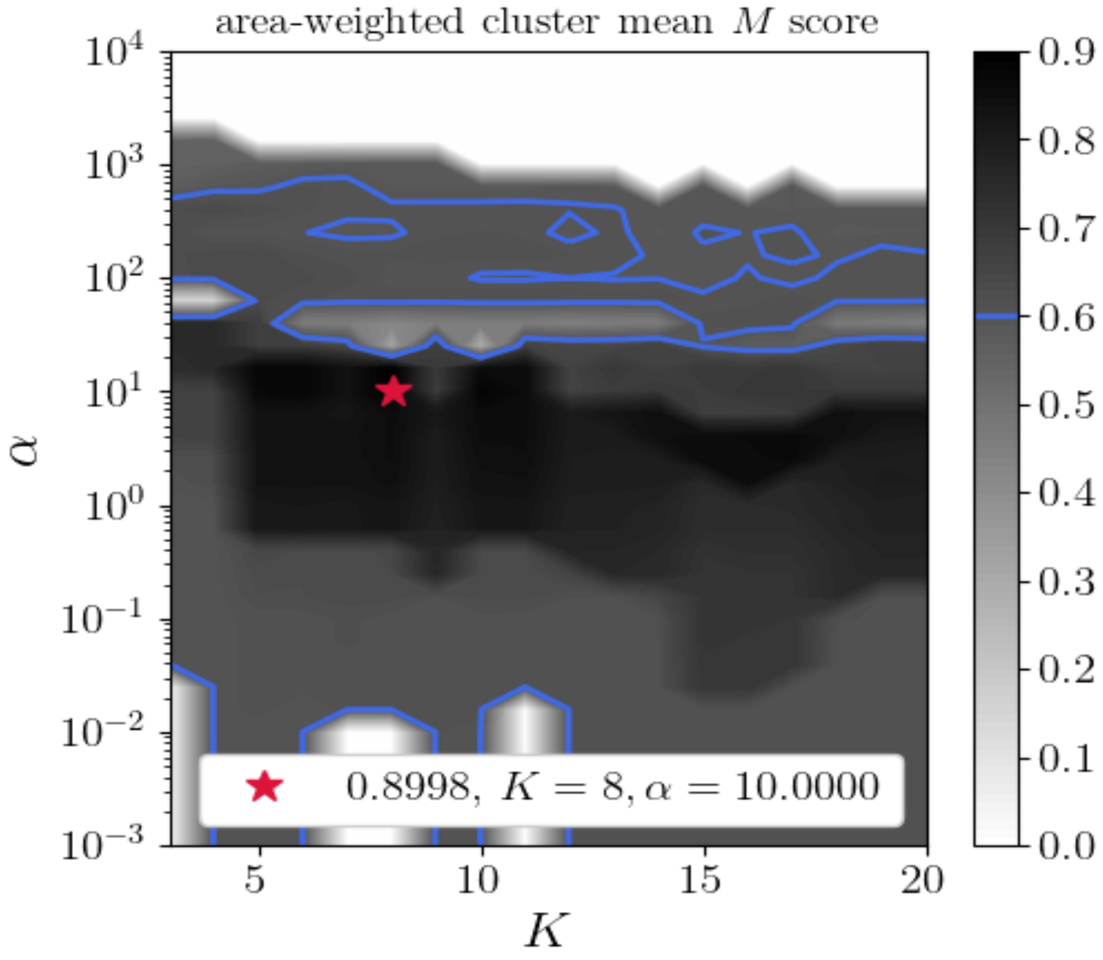


5. Results: optimization over free parameters

Gaussian Mixture Model (GMM) clustering



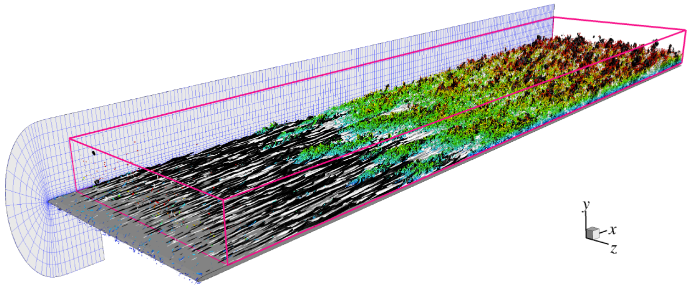
Combinatorial Hypothesis Selection (CHS)
for identification & agglomeration

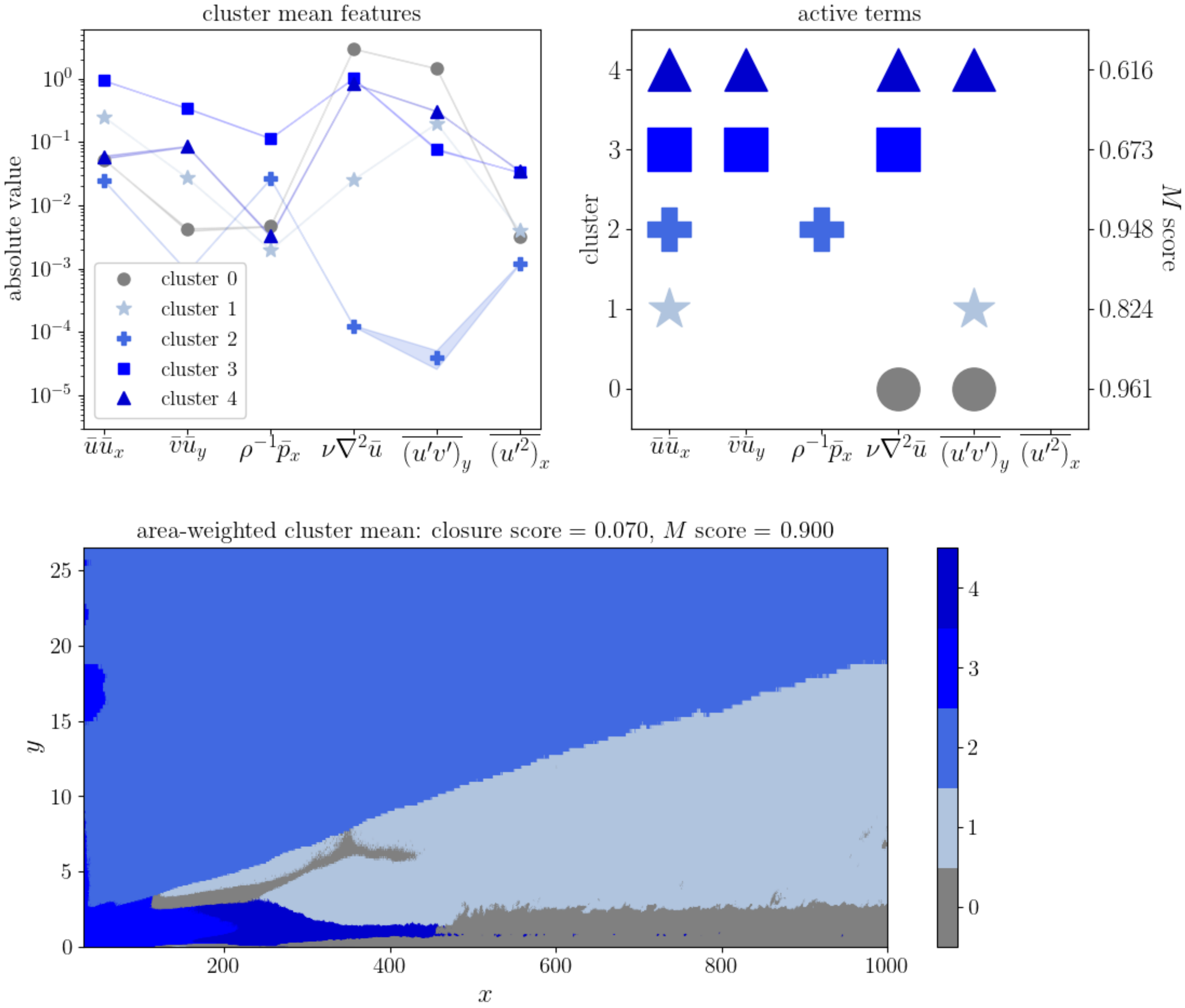


SPCA
for identification & agglomeration
(method of Callaham et al. 2020)

5. Results

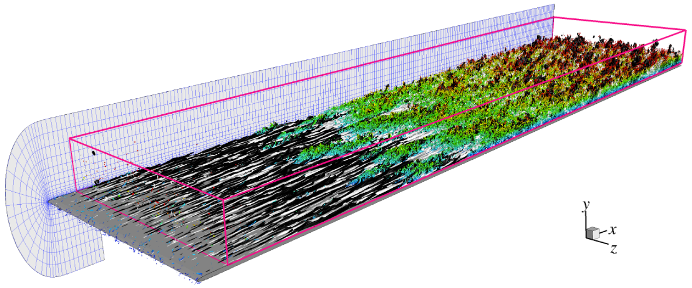
GMM clustering
+
SPCA

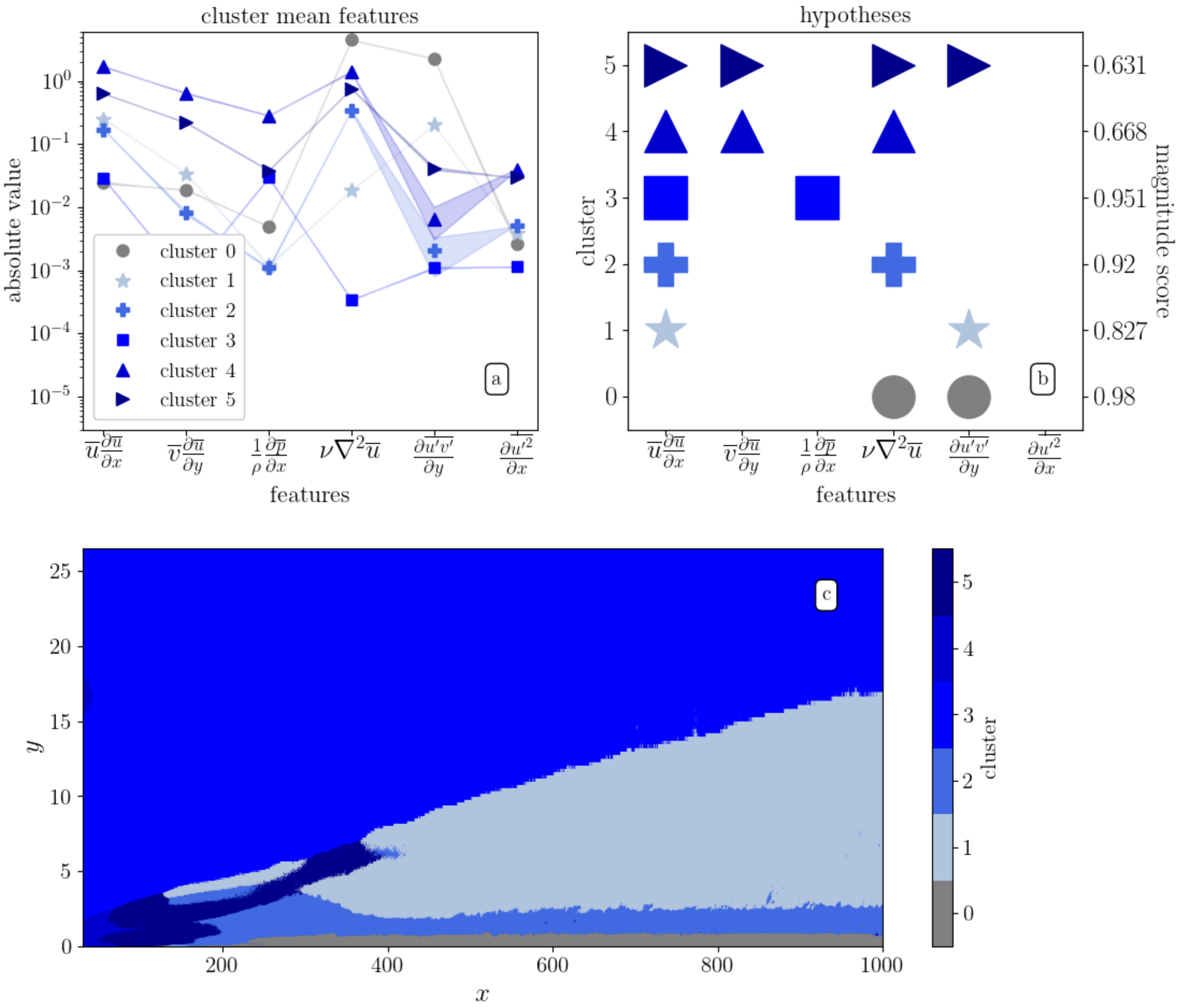




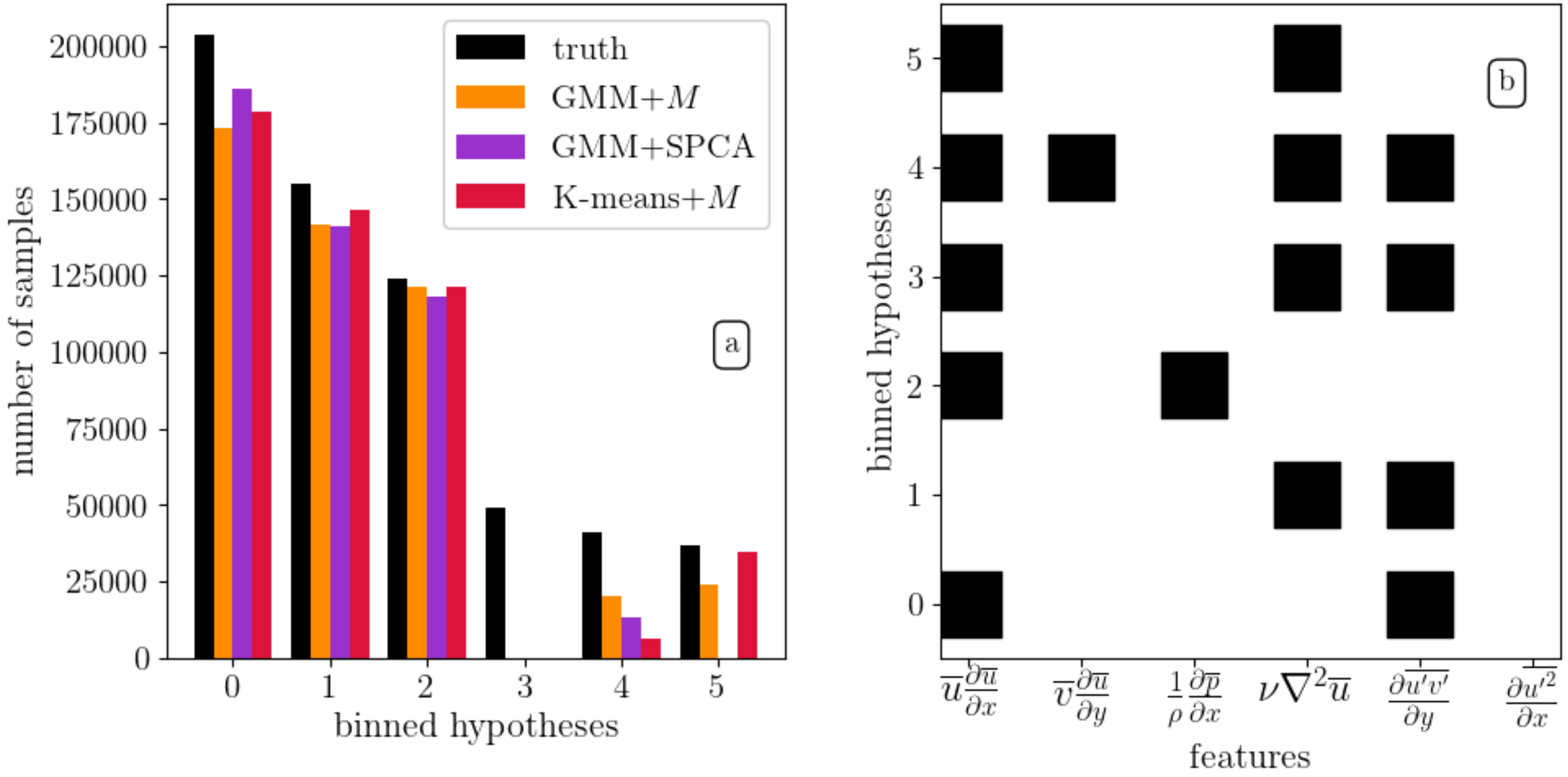
5. Results

GMM clustering
+
CHS identification and agglomeration





5. Results: comparison to no clustering



6. Conclusions

- By combining the CHS algorithm with a clustering algorithm, leading-order analysis can transformed into an optimization problem.

- The determination of an appropriate characteristic feature vector for each cluster may be a direction for future work.

- This algorithm could be combined with PDE-modeling algorithms to create an AI dynamical modeler.

- Thank you for listening + questions!

Image credit: NASA